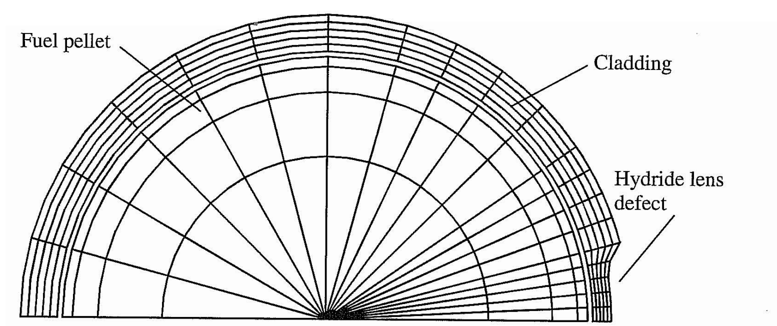
Existing Fuel Performance Models

LWR Fuel Behavior Modeling – U.S. State of the Art

- Code development efforts have been limited since the early 80's
- **FRAPCON** (non-proprietary)
  - 1.5 D finite difference
  - steady operation (separate code for transients)
  - highly empirical
  - highly simplified fuel mechanics
- **FALCON** (proprietary – EPRI owned; developed by ANATECH)
  - 1.5 or 2D (R-Z or R-q) FEM with coupled thermomechanics
  - steady and transient operations
  - contact with friction and sliding
  - smeared-crack constitutive behavior



FALCON model to investigate clad failure due to defect

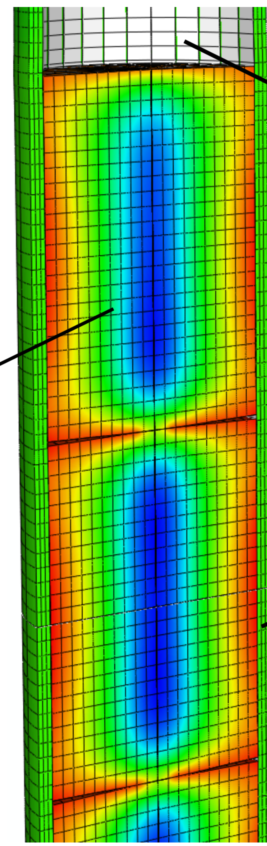
Fuel Performance Models

- Coupled thermomechanics model describes fuel rod behavior

Heat Conduction: $\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + E_f \dot{F}$ *Mechanics:* $\nabla \cdot \mathbf{T} + \rho \mathbf{f} = 0$

- Microstructure evolution is described by materials models

Fuel Behavior
- Volumetric heat generation (fission)
- Thermal conductivity is a function of:
  - Temperature
  - fission products
  - Off-stoichiometry
  - Porosity
  - Radiation damage
- Volumetric strain:
  - Densification
  - Solid and gaseous fission products
- Pressure increase due to fission gas release



Gap/Plenum Behavior
- Gap heat transfer with k_g= f (T, n)
- Mechanical contact
- Plenum pressure as a function of:
  - evolving gas volume (from mechanics)
  - gas mixture (from FGR model)
  - gas temperature approximation

Cladding Behavior
- Thermal and irradiation creep
- Thermal expansion
- Plasticity

Unirradiated Thermoconductivity

- Changes with temperature
- Fink model accurate description of how k_0 changes with temperature

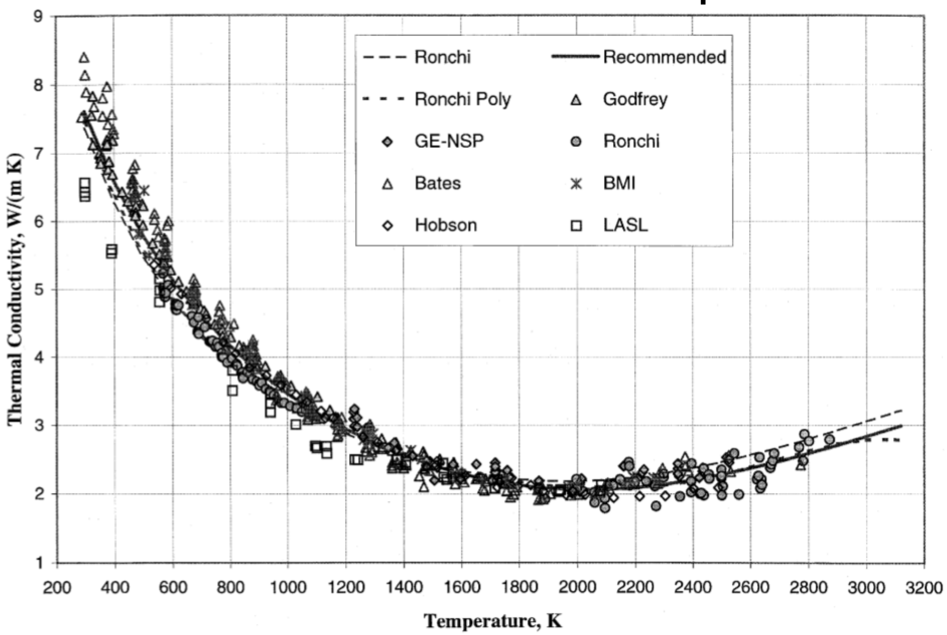


Fig. 9. Comparison of the recommended equation for the thermal conductivity of 95% dense UO_2, Eq. (19) with the data fit and the equations of Ronchi et al. [5] (physically based Eq. (16) and polynomial fit to their measurements).

$$k_0 = \frac{100}{7.5408+17.629t+3.6142t^2} + \frac{6400}{t^{5/3}} \exp\left(\frac{-16.35}{t}\right)$$

J.K. Fink, J. Nucl. Mater. 279 (2000) 1-18

Effect of Radiation on Thermoconductivity

- Microstructural changes that take place within the fuel during its lifetime in a reactor degrades the thermoconductivity, including
  - Solid fission products, dissolved and precipitated
  - Pores and fission gas bubbles
  - Oxygen off-stoichiometry
  - Radiation damage

Une et al., J. Nucl. Mater. (2000)

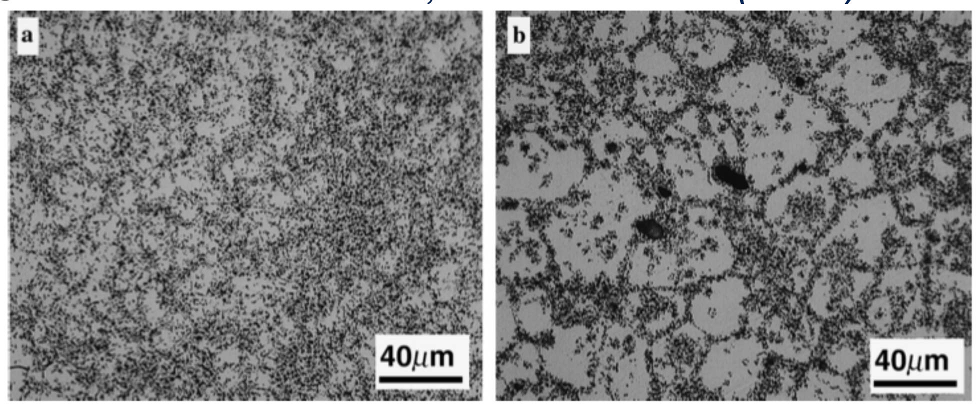


Fig.11. Ceramographs at $r/r_o = 0.74$ on as-etched surface of fuels irradiated to 86 GWd/t in IFA566 rig: (a) standard fuel, (b) Al–Si–O doped large-grained fuel.

- Lucuta et al. proposed a multiplicative decomposition of the various effects $k = \kappa_{fp}\,\kappa_p\,\kappa_{O/M}\,\kappa_{rd}\,\kappa_{cr}\,k_0$

Lucuta Model

Lucuta, J Nuc Mat, 232 (1996) 166

- Using SIMFUEL (simulated high-burnup fuel), the effects of fission products and off-stoichiometry were determined using empirical fits

$$\kappa_{1p} = 1 + \frac{0.019\beta}{(3 - 0.019\beta)} \frac{1}{1 + \exp(-(T - 1200)/100)}$$

$$\kappa_{1d}(\beta) = \left(\frac{1.09}{\beta^{3.265}} + \frac{0.0643}{\sqrt{\beta}}\sqrt{T}\right)$$

$$\arctan\left(\frac{1}{1.09/\beta^{3.265} + \left(0.0643/\sqrt{\beta}\right)\sqrt{T}}\right)$$

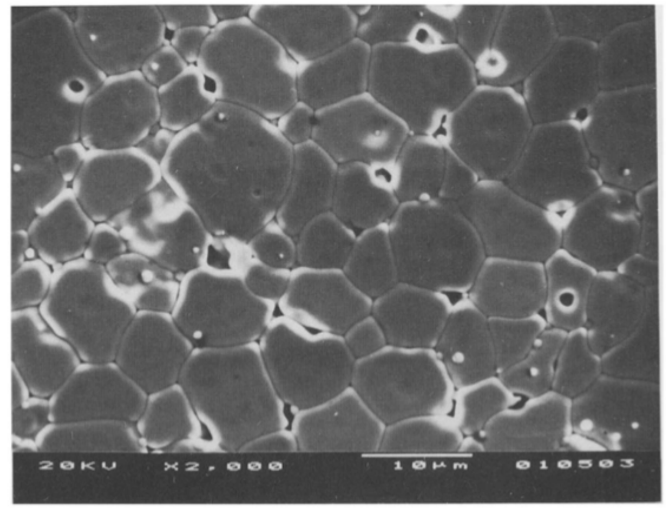


Fig. 1. SEM image of a polished and etched surface of 6 at% burnup SIMFUEL showing equiaxed matrix grains and precipitates.

$$\frac{1}{k_{2+x}} = \frac{1}{k_0} + \frac{1}{k_x} = (a_0 + a_1 x) + (b_0 - b_1 x)T$$

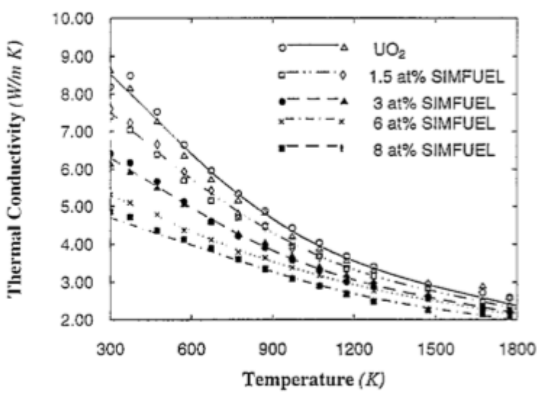


Fig. 2. Thermal conductivity of fully dense UO_2 and SIMFUEL with an equivalent burnup of 1.5, 3, 6 and 8 at.% as a function of temperature [16–19].

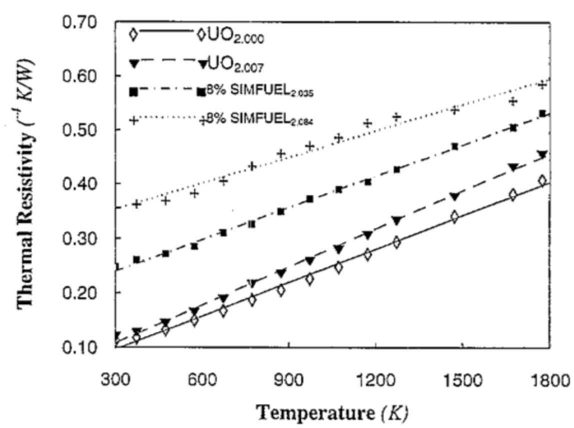


Fig. 5. The effect of deviation from stoichiometry in UO_{2+x} and SIMFUEL for the thermal resistivity plotted as a function of the temperature [21].

Lucuta Model (cont)

- Effects of porosity and radiation damage on thermal conductivity were taken from the literature
  - Porosity effect taken from Maxwell-Eucken formula $\kappa_{2p} = \frac{1-p}{1+(\sigma-1)p}$
    - Analytical formula
    - Assumes uniform porosity distribution
    - Pore shape accounted for with shape factor, σ
    - Experimental data showing the effect of porosity for high porosities is not available
  - Radiation damage
    - From an empirical study
    - Considers point defect effect

$$\kappa_{4r} = 1 - \frac{0.2}{1+\exp((T-900)/80)}$$

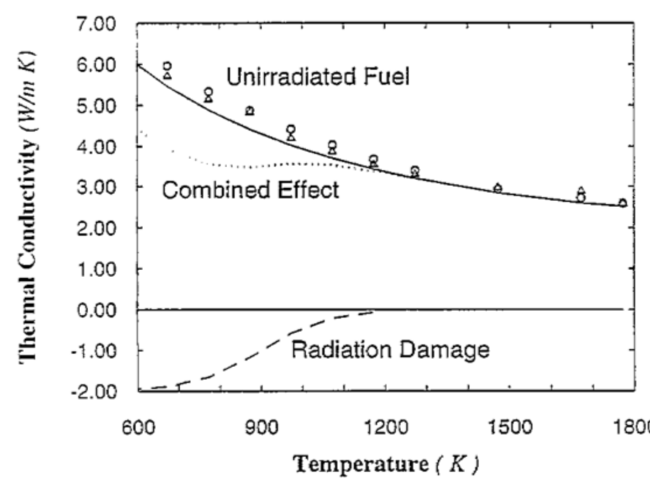


Fig. 8. Estimated effect of radiation damage on fuel thermal conductivity and the overlapped effect as a function of the temperature.

Unirradiated Thermal Expansion

- Significant thermal expansion occurs within the fuel due to the high temperatures
- Data is summarized and best fit model is presented in Fink (2000)

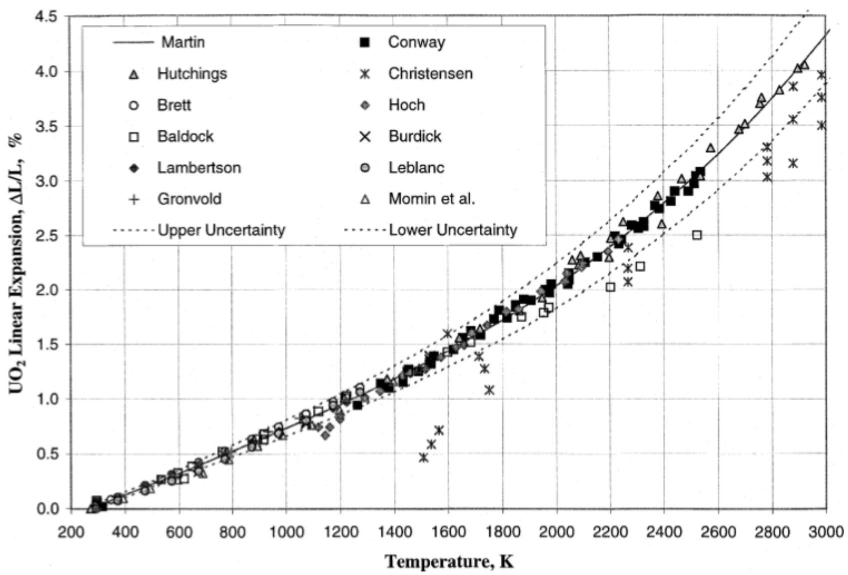


Fig. 5. Measurements of the linear expansion, $\Delta L/L$, of solid UO_2 compared with the recommended equation of Martin [40] and its recommended uncertainties.

$$\alpha_P(l) = \frac{1}{L}\left(\frac{\partial L}{\partial T}\right)_P. \quad (9)$$

For 273 K $\leqslant T \leqslant$ 923 K,

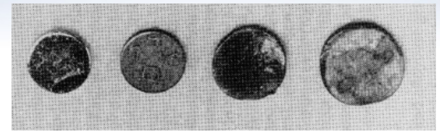
$$\alpha_P(l) = 9.828 \times 10^{-6} - 6.930 \times 10^{-10} T + 1.330 \times 10^{-12} T^2 - 1.757 \times 10^{-17} T^3; \quad (10)$$

for 923 K $\leqslant T \leqslant$ 3120 K

$$\alpha_P(l) = 1.1833 \times 10^{-5} - 5.013 \times 10^{-9} T + 3.756 \times 10^{-12} T^2 - 6.125 \times 10^{-17} T^3, \quad (11)$$

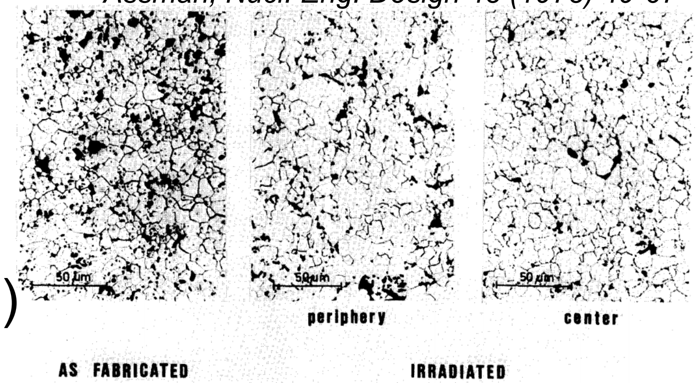
J.K. Fink, J. Nucl. Mater. 279 (2000) 1-18

Other Volumetric Strains



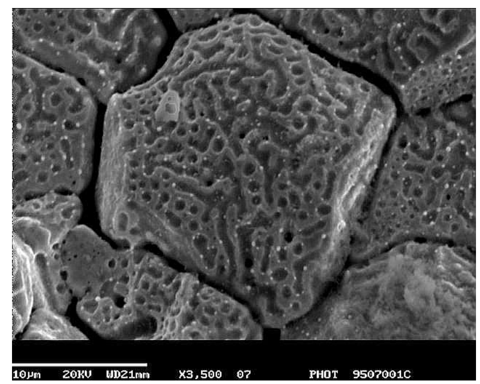
- Additional volumetric strains occur in reactor:
  - Densification early in the fuel life
  - Solid and gaseous fission product swelling

Assman, Nucl. Eng. Design 48 (1978) 49-67



- Densification (MATPRO empirical correlation)

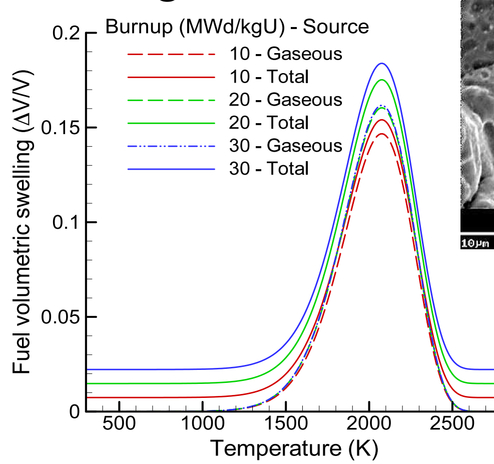
$$\varepsilon_D = \Delta\rho_0 \, e^{\frac{Bu \ln(0.01)}{C_D Bu_D}} - 1$$



- Solid and gaseous fission product swelling (MATPRO empirical correlations)

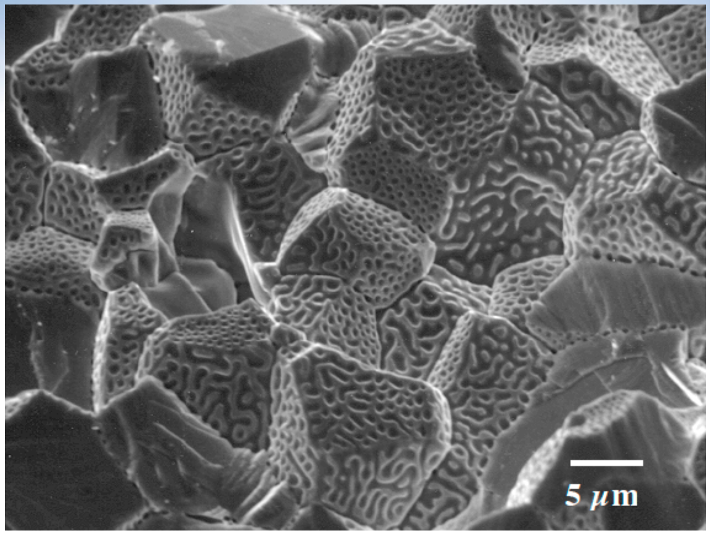
$$\Delta\varepsilon_{sw-s} = 6.407x10^{-5} \rho \, \Delta Bu$$

$$\Delta\varepsilon_{sw-g} = 2.25x10^{-31} \Delta Bu \; \rho \; (2800 - T)^{11.73} \; * \; e^{-0.0162\,(2800-T)} \; e^{-0.021\,\rho\, Bu}$$



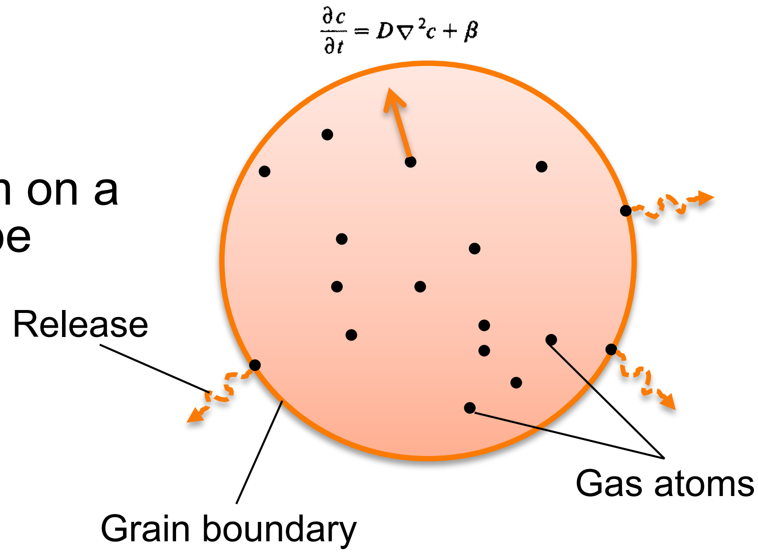
Fission Gas Release

- Fission gas is released into the gap and plenum after three steps
  1. Diffusion of gas from grain interior to grain boundaries
  2. Coalescence of bubbles to triple junctions
  3. Percolation of bubbles over various grains until they reach a free surface

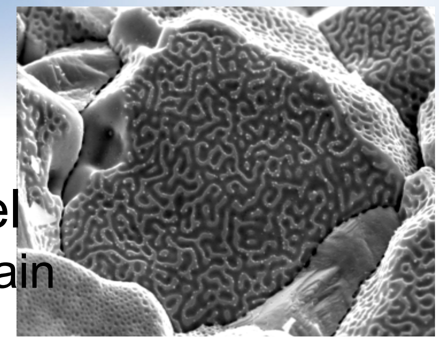


- Booth Model
  - Only considers diffusion of gas to grain boundaries (step 1)
  - Diffusion controlled model; any gas atom on a grain boundary is assumed to instantly be released

$$f_c = 4\left(\frac{\omega}{\pi}\right)^{1/2} - \frac{3}{2}\omega$$

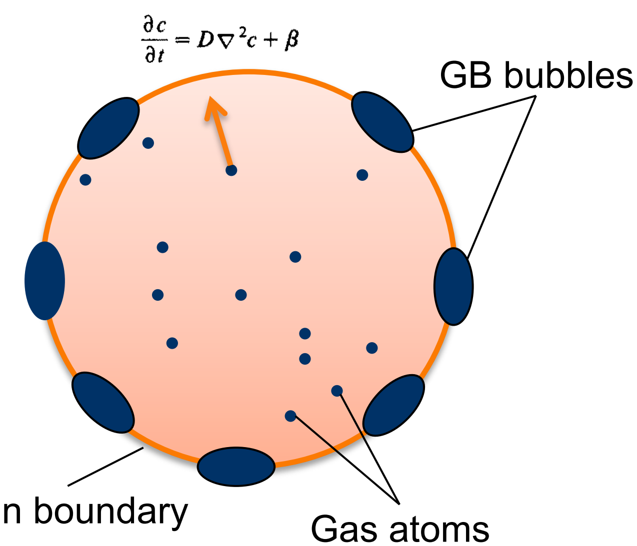


Fission Gas Release (cont)



- Two stage Forsberg-Massih mechanistic model
  - Considers intragranular diffusion diffusion to grain boundaries (step 1)
  - Also, grain boundary gas accumulation, resolution back into grain, saturation (step 2)
  - Assumes that once the porosity on a bubble is interconnected, it is released

Fission gas is released once the GB coverage reaches a predetermined threshold



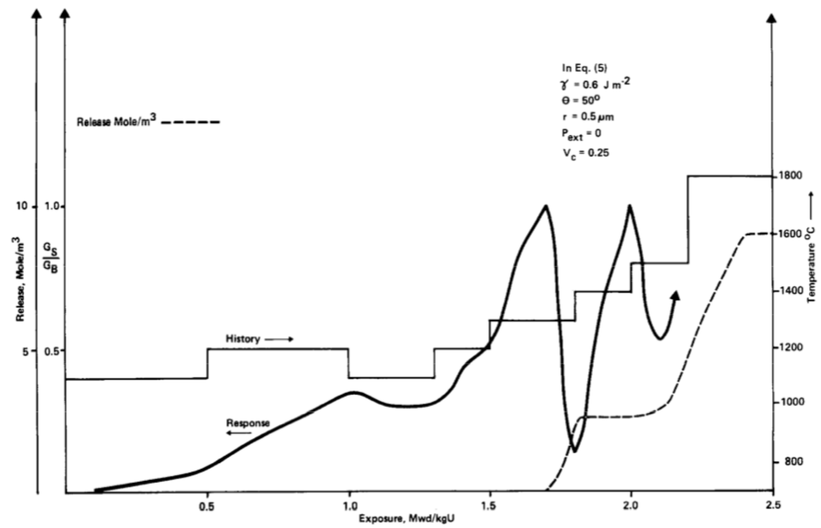
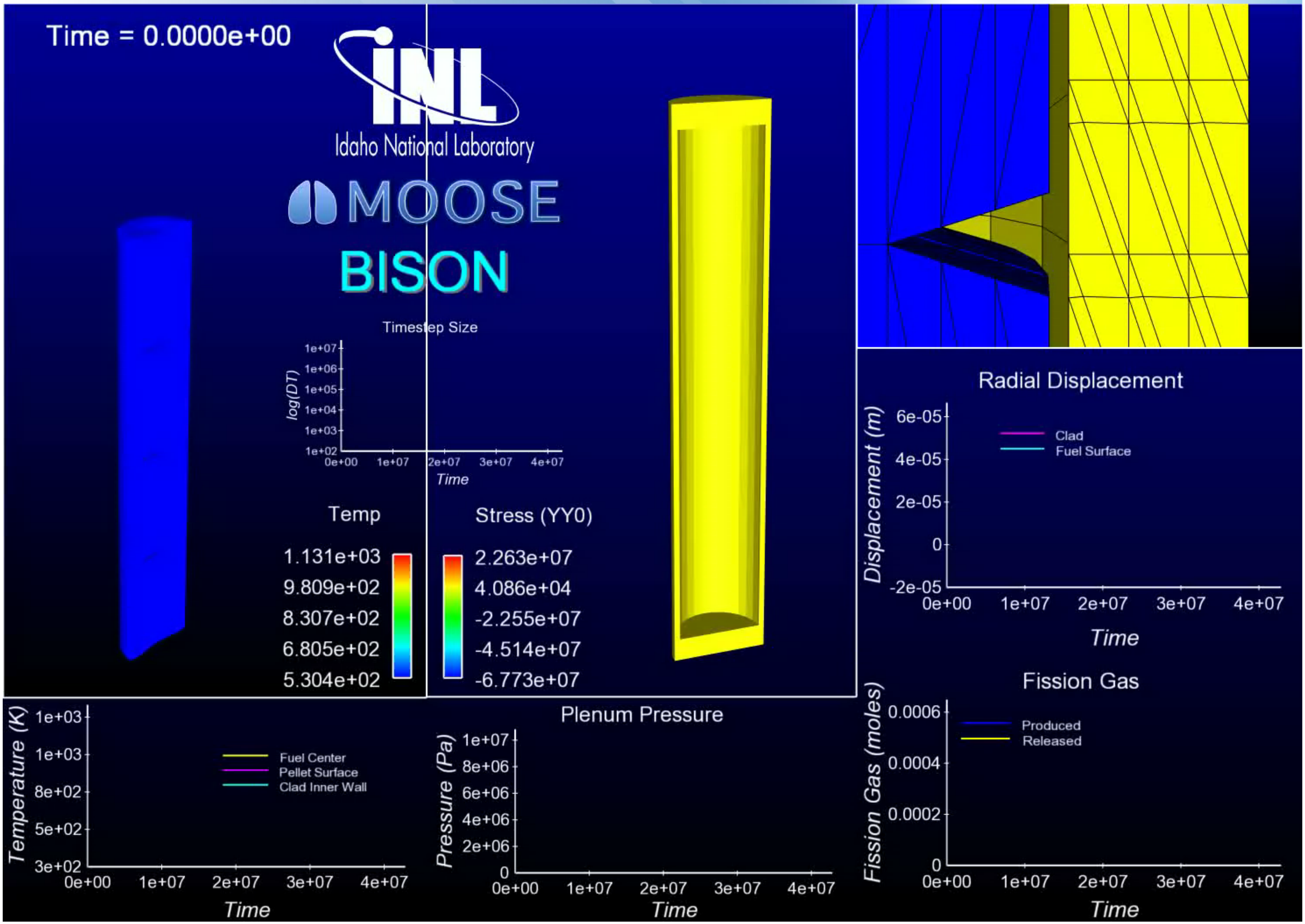


Fig. 1. Fraction of gas atoms on grain boundary, G_s/G_B, as a function of exposure for downward fuel cascading temperature history. γ is the bubble surface tension, 2θ is the angle where two free surfaces meet at a grain boundary, r is average bubble radius, V_c is the fractional coverage of the grain boundaries at saturation and the grain radius is taken to be 5 μm.

Forsberg & Massih, J. Nucl. Mater. 135 (1985) 140-148



Time = 0.0000e+00
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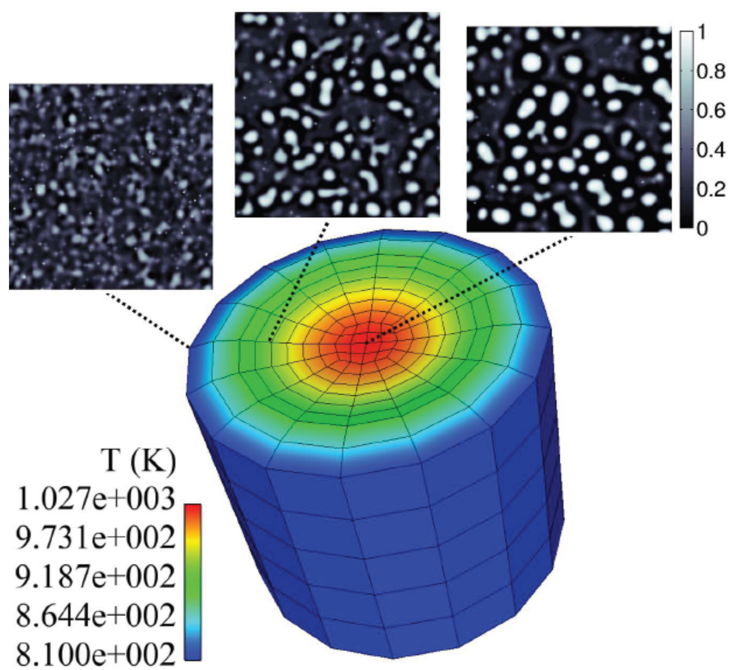
MOOSE
BISON
Timestep Size
log(DT)
Time
Temp
1.131e+03
9.809e+02
8.307e+02
6.805e+02
5.304e+02
Stress (YY0)
2.263e+07
4.086e+04
-2.255e+07
-4.514e+07
-6.773e+07
Radial Displacement
Displacement (m)
Clad
Fuel Surface
Time
Fission Gas
Fission Gas (moles)
Produced
Released
Time
Temperature (K)
Fuel Center
Pellet Surface
Clad Inner Wall
Time
Plenum Pressure
Pressure (Pa)
Time

Issues with Traditional Models

- Empirical or semi-empirical models cannot accurately be extrapolated to new conditions or materials
- Some simplifying assumptions are incorrect
- Coupled behaviors are treated as uncoupled
  - e.g. Fission gas effect on thermal conductivity is treated separately from the fission gas effect on swelling and both are separate from the fission gas release model.
- Hard to measure behaviors are treated with simple analytical models that have not been verified

Multiscale Fuel Performance Model Approach

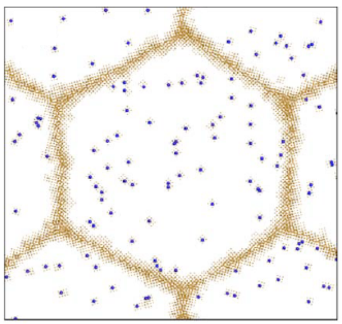
Simulations at various scales are used to improve and replace traditional materials models



New Multiscale Modeling Approach

- Empirical models can accurately interpolate between data but cannot extrapolate outside of test bounds
- *Research goal: To develop improved, science-based materials models for fuel performance using hierarchical multiscale modeling*

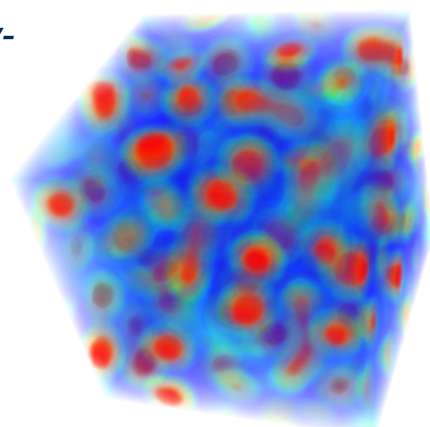
Atomistic simulation



- Atomic scale resolution of material behavior
- Extremely limited on length and time scales

Atomistically-informed parameters

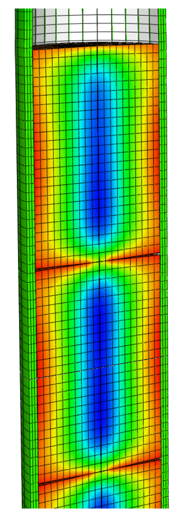
Mesoscale models



- Describes microstructure evolution
- Limited to micron length scales

Mesoscale-informed materials models

Fuel performance models

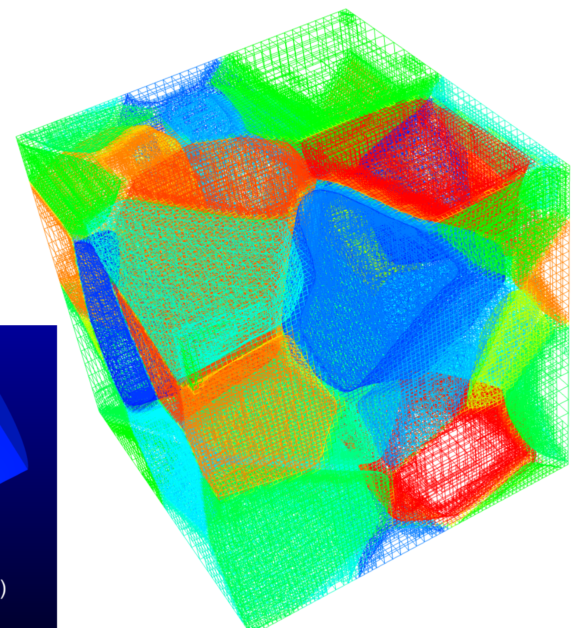


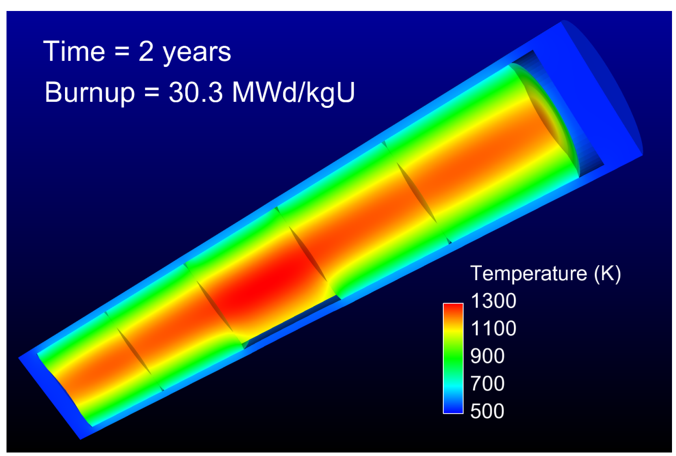
- Models fuel rods/ fuel assemblies

Simulation results will be validated with experiments

Scale-Bridging to Macroscale

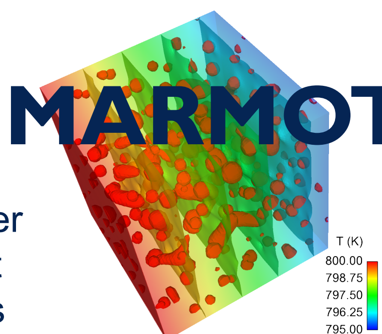
MBM: Multiscale Fuel Performance Code

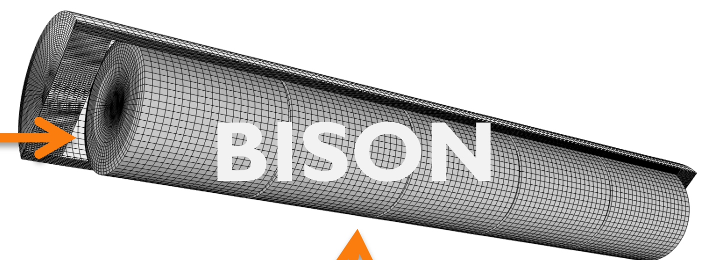




MBM Summary

- MBM (MOOSE-BISON-MARMOT) is a NEAMS-funded fuel performance code
- Objective: To deliver a science-based (truly predictive) computational tool for nuclear fuel pin analysis and design





Bulent Biner
Paul Millett
Mike Tonks
Karthik Chockilingham
Liangzhe Zhang
Yongfeng Zhang

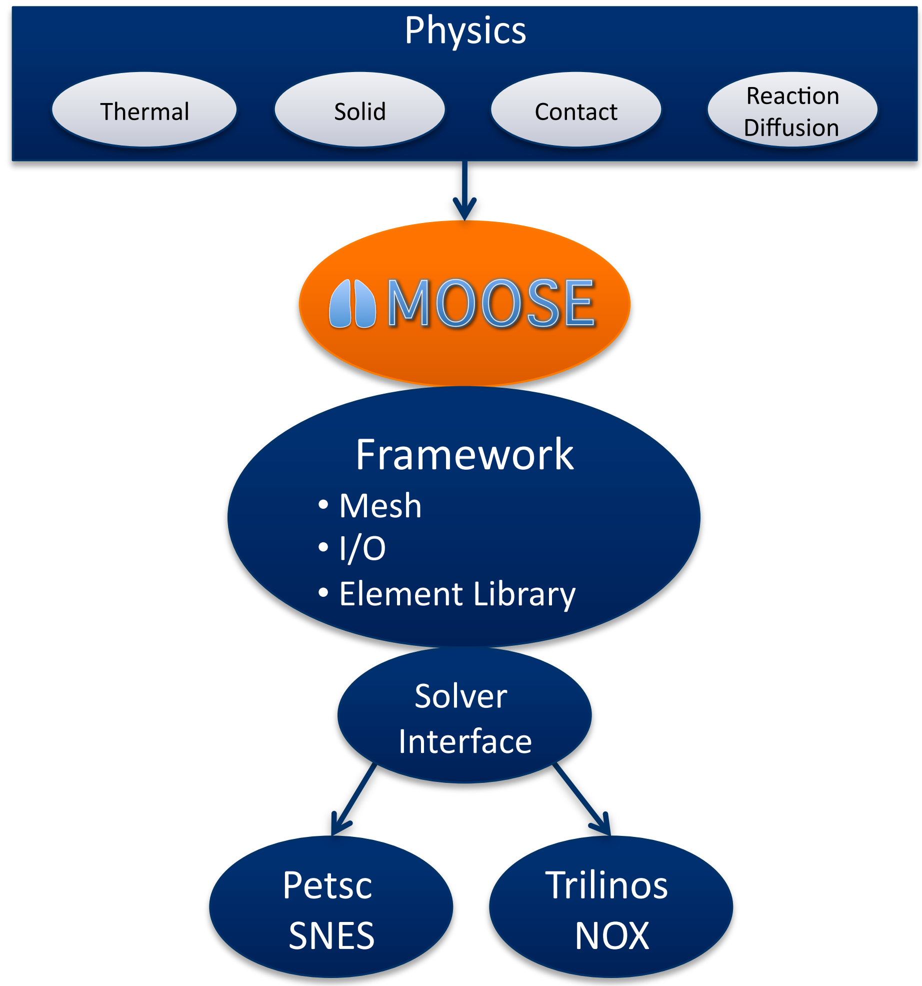
Richard Williamson
Jason Hales
Steve Novascone

MOOSE

Derek Gaston
Cody Permann
David Andrs
John Peterson

Multiscale Object Oriented Simulation Environment (MOOSE)

- Finite element-based partial differential equation solver in 1-, 2- and 3-D
- User only required to create objects to define the physics
- Parallel framework provides core set of common services
  - libMesh: http://libmesh.sf.net
- Fully-coupled multiphysics using Jacobian-Free Newton Krylov
- Utilizes state-of-the-art linear and non-linear solvers
  - Robust solvers are key for "ease of use"



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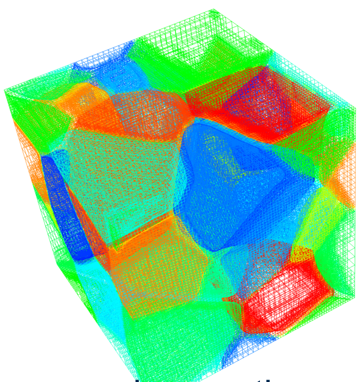
MARMOT

- Determine microstructure evolution due to applied load, temperature gradients and radiation damage.

Technique: Phase field with solid mechanics and heat conduction

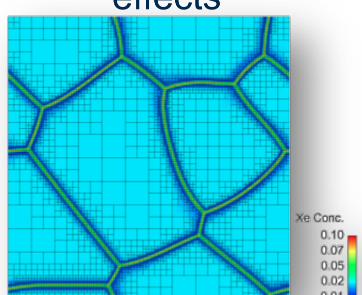
Solution method: Implicit finite element

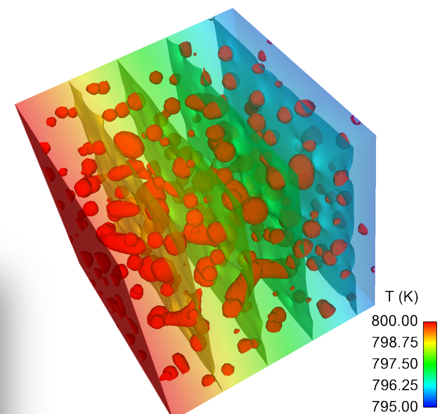
Physical phenomena:



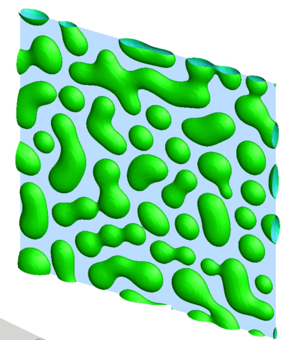
grain growth, stress effects

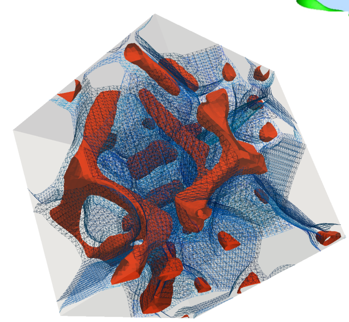
Grain boundary effects





Void nucleation, effect on heat conduction

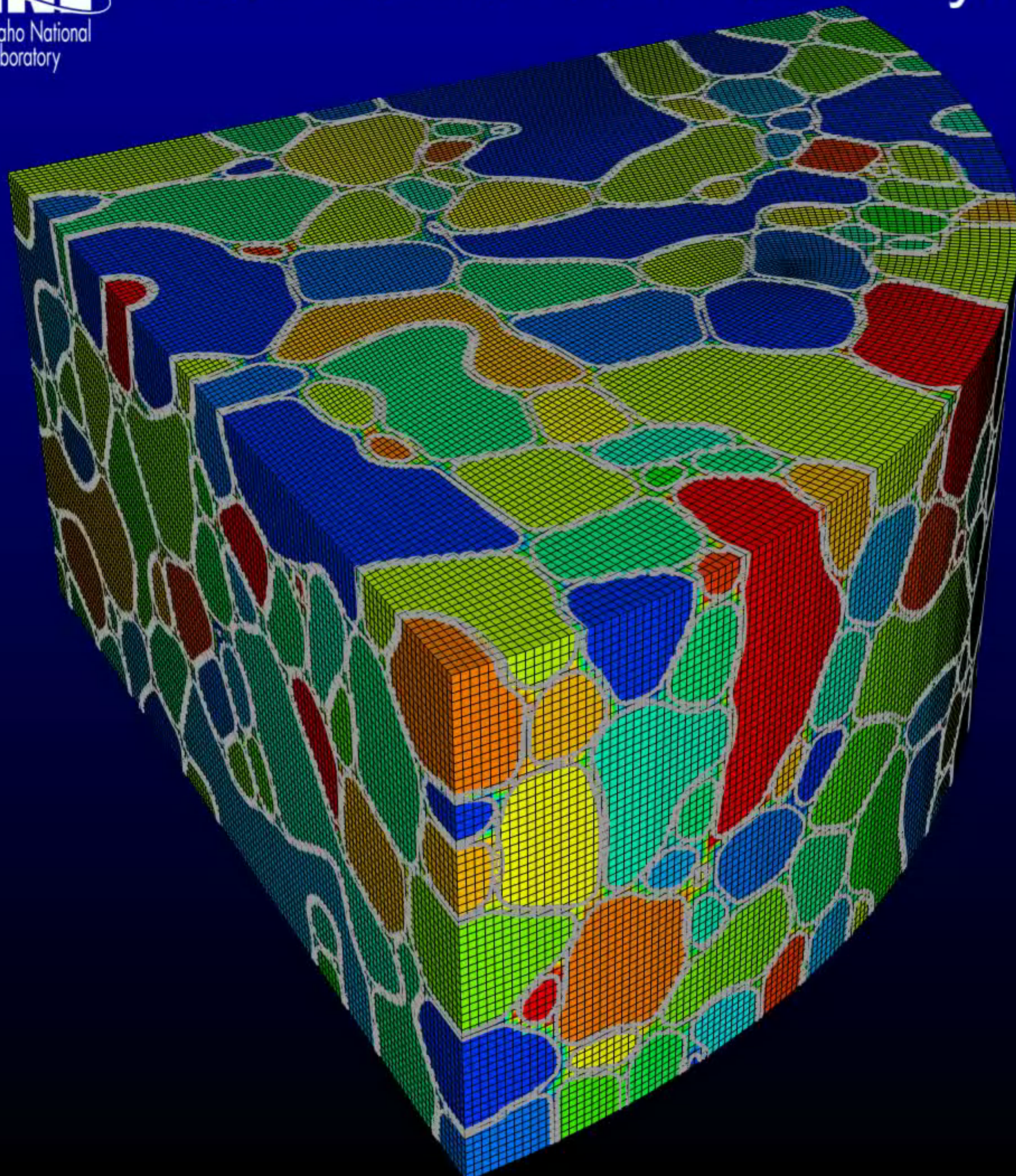




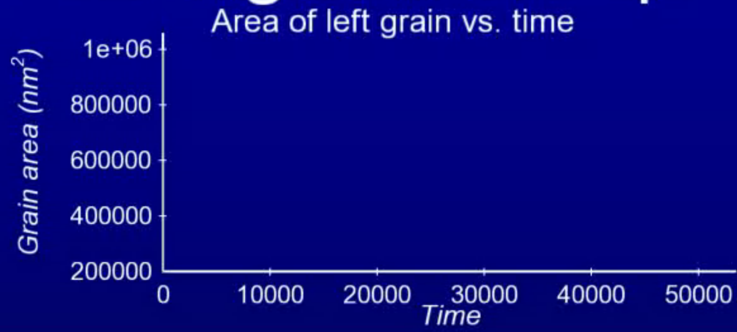
Bubble growth and percolation

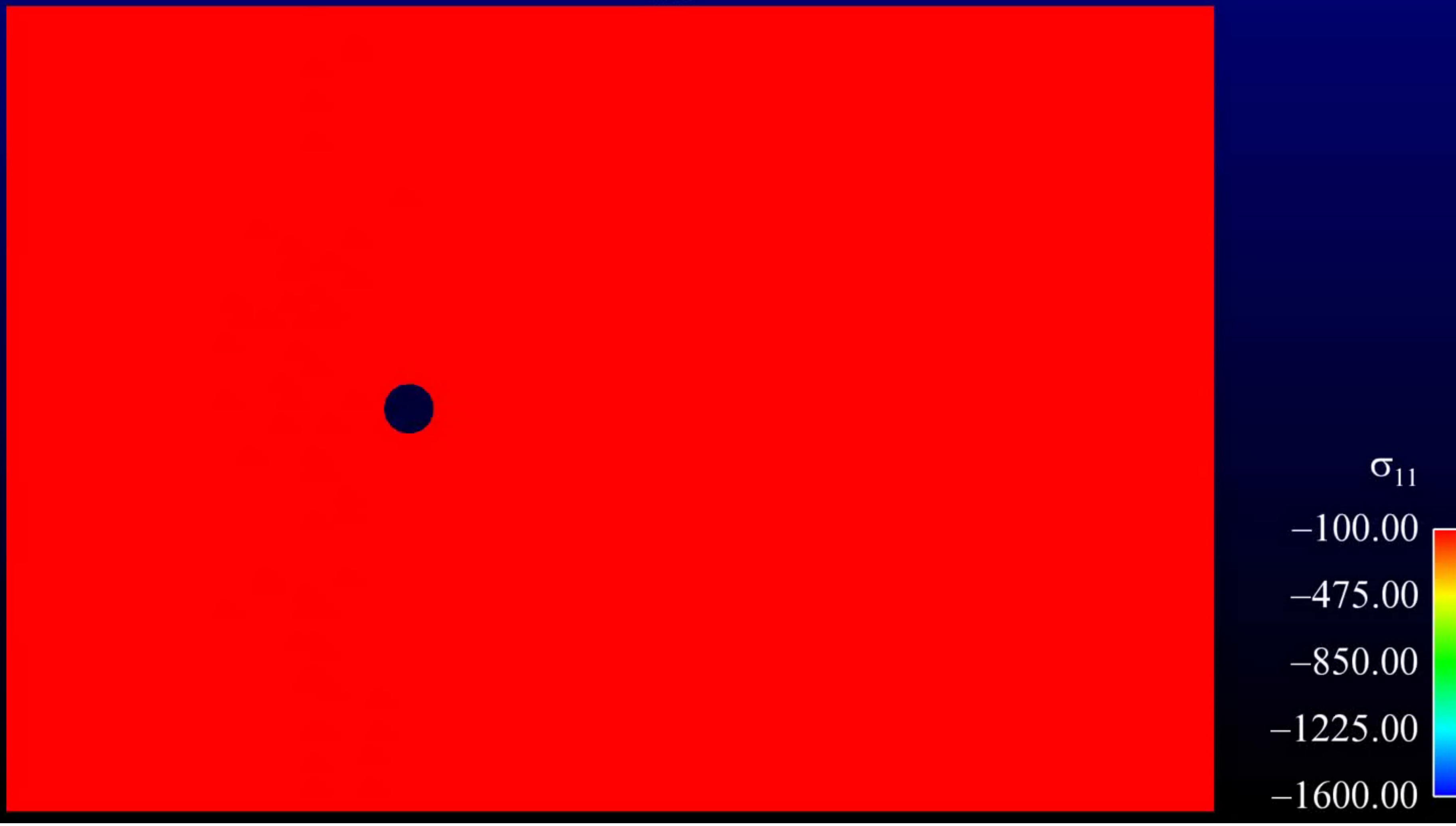
Models to be validated with experiments, including diffusion couples, post-irradiation annealing, and ion and neutron irradiations. SEM, TEM, Laser resonant ultrasound spectroscopy, positron annihilation spectroscopy, etc. will be used to gather data

Grain Growth in a Small Cylinder

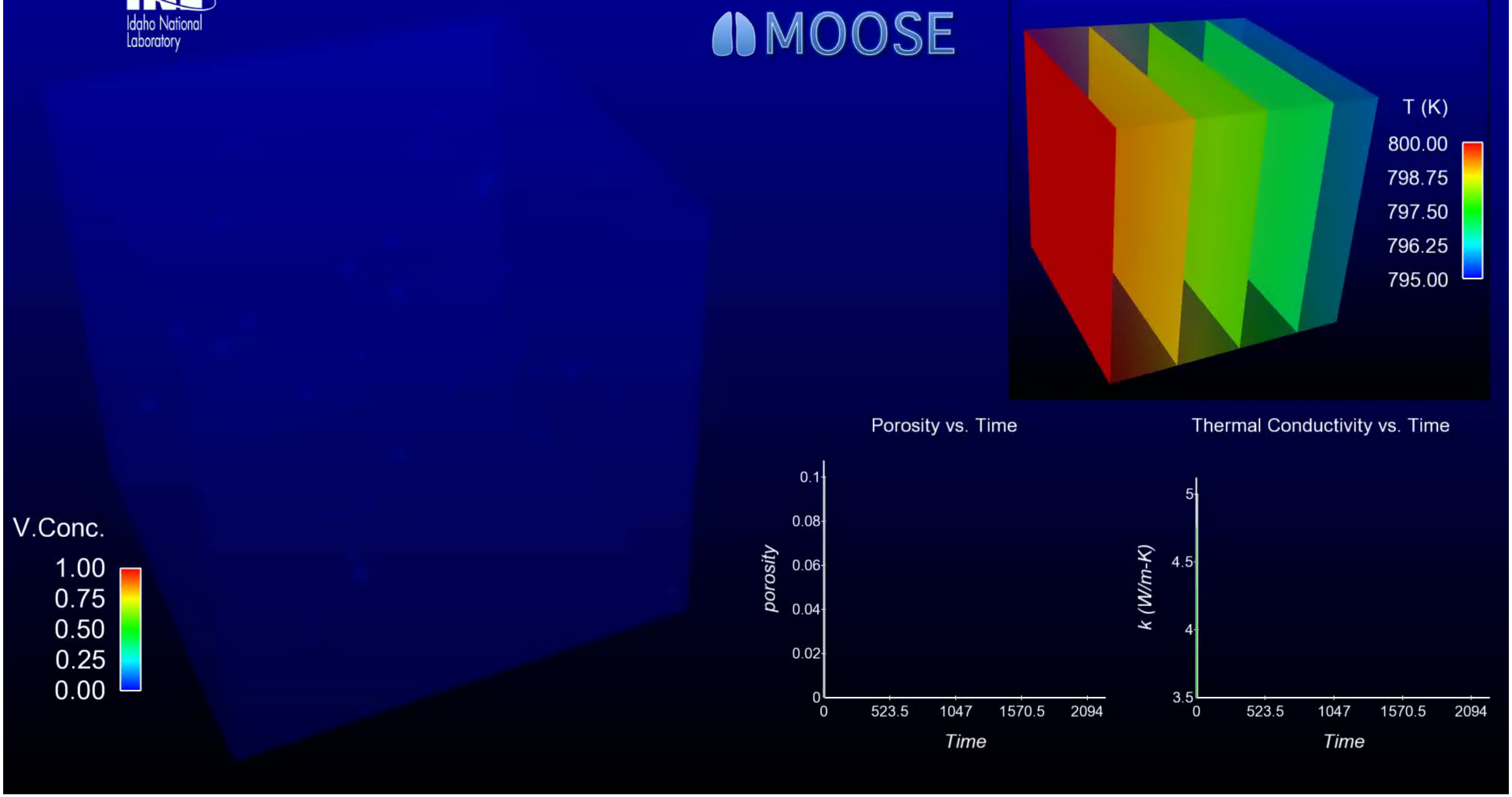


Void Pinning in a Compressed Bicrystal



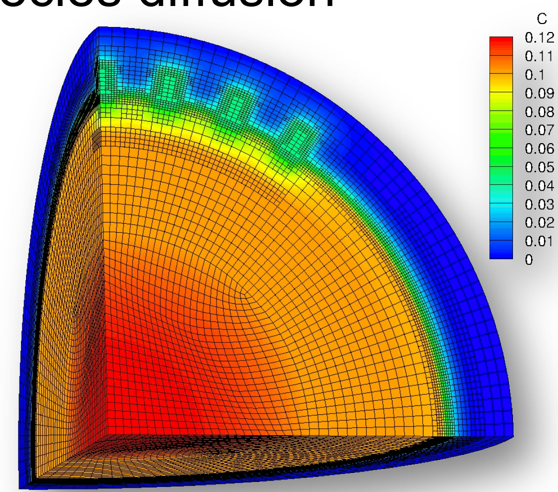


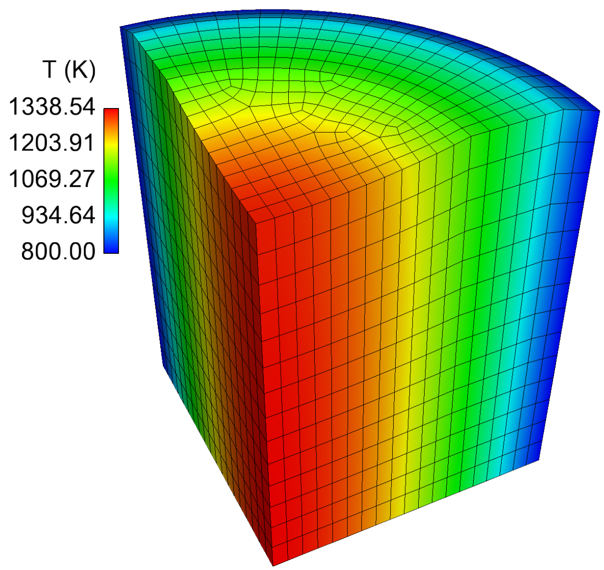
The Effect of Void Formation on Thermal Conductivity

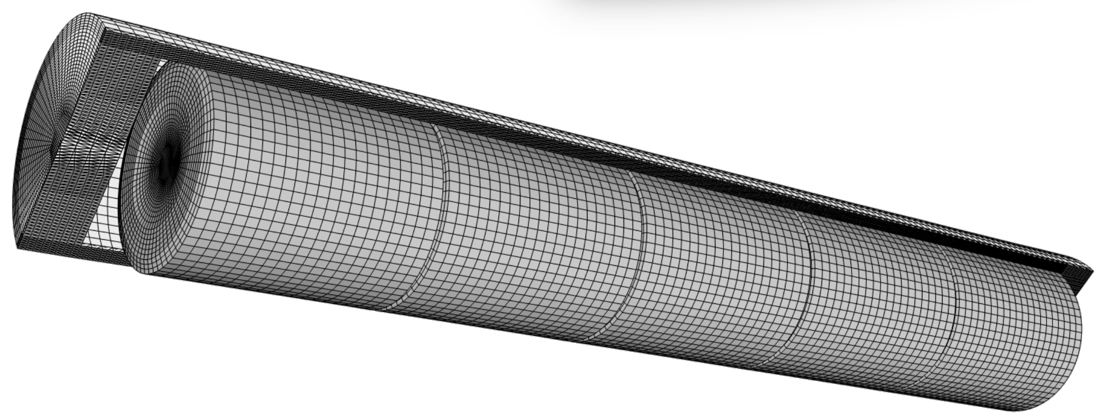


BISON

- Solves the fully-coupled thermomechanics and species diffusion equations in 1D-3D
- Includes multiphysics constitutive behavior
- Applicable to both steady and transient operation
- Massively parallel computers
- Applicable to LWR, TRISO, and TRU fuel







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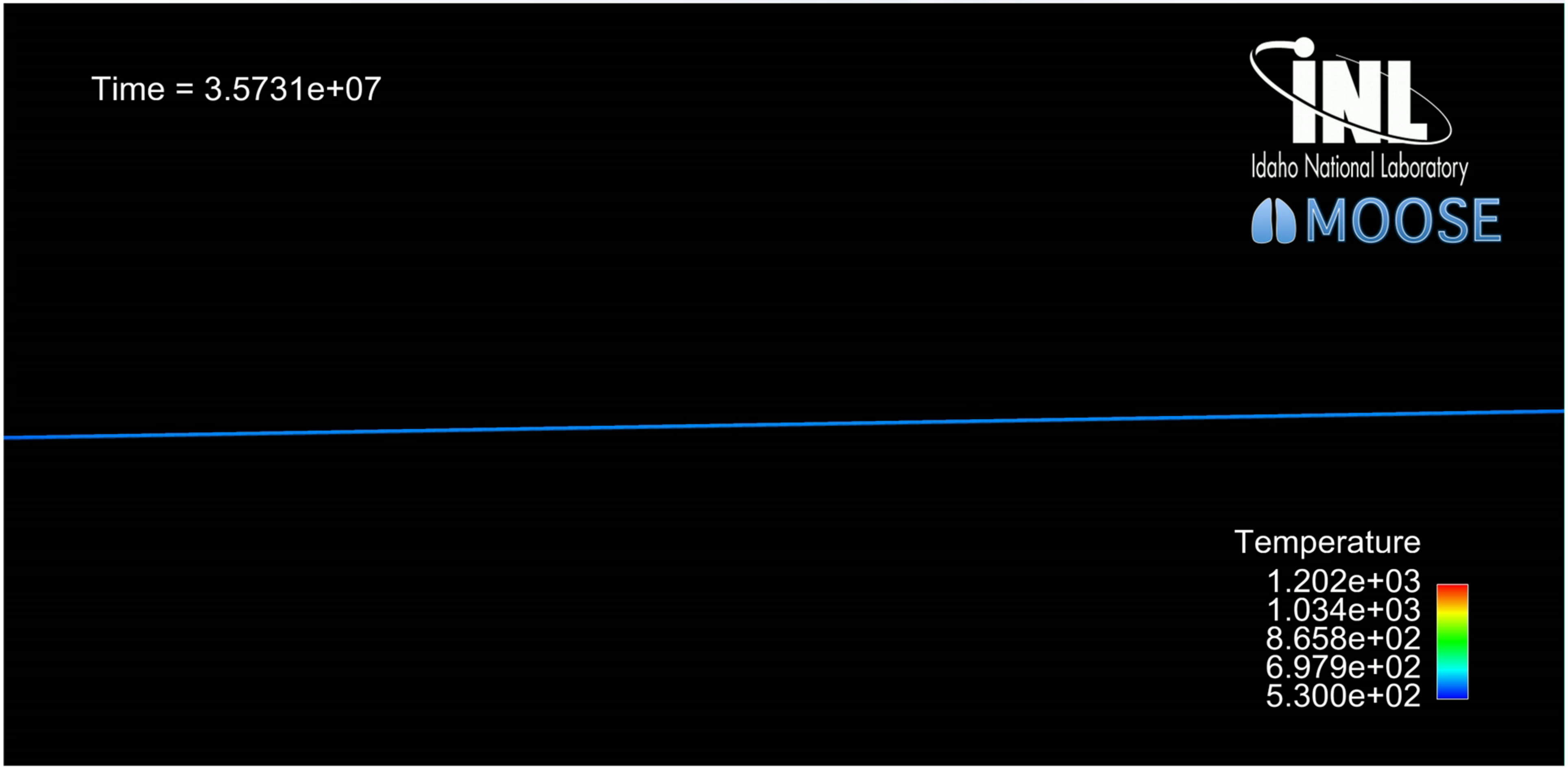
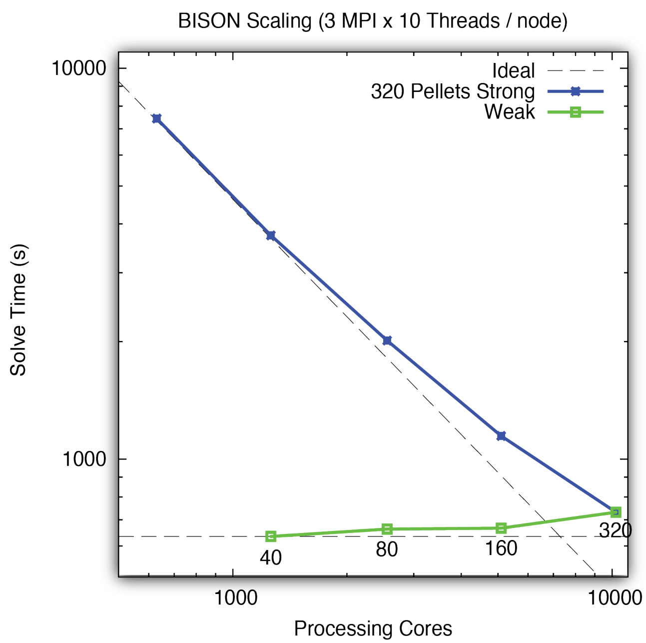
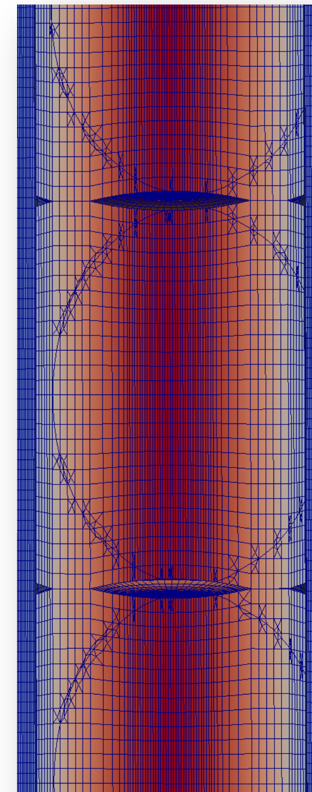
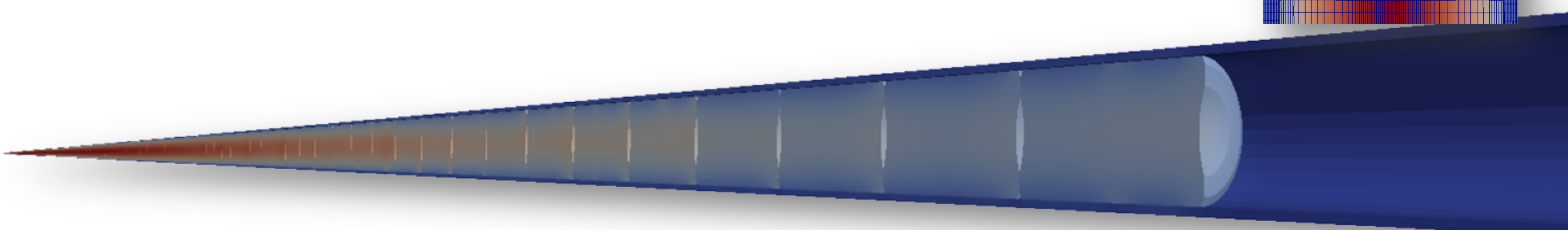


Full Fuel Pin Simulation



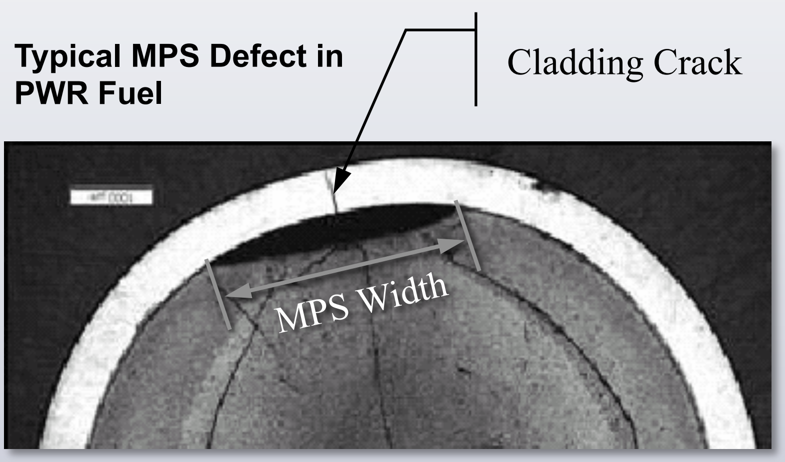
- **First 3-D full fuel pellet simulation**
- 320 pellets with 234M degrees of freedom
- Massively parallel (tested using up to 11,820 cores)
- Good weak and strong scaling over 10K cores using fully implicit time integration and fully-coupled multiphysics

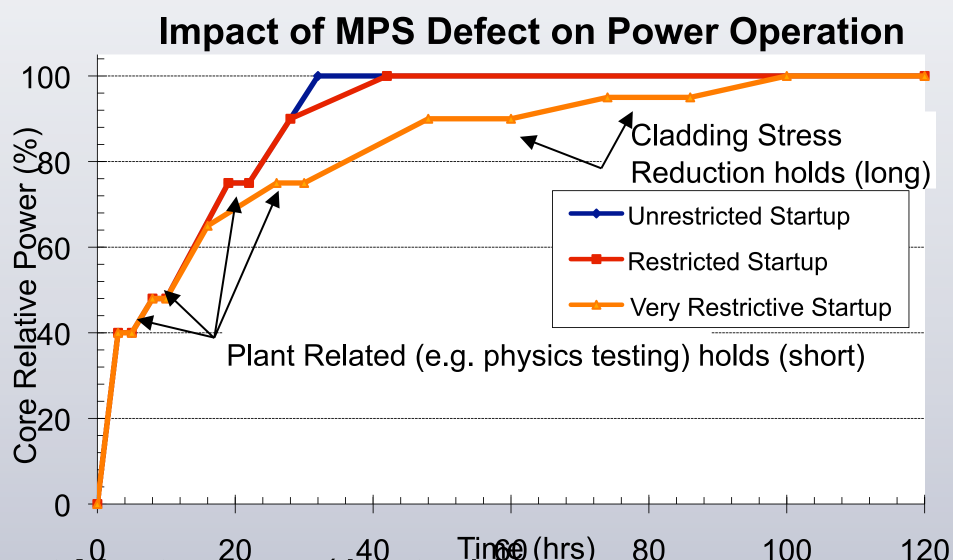




3-D Simulation of Missing Pellet Surface

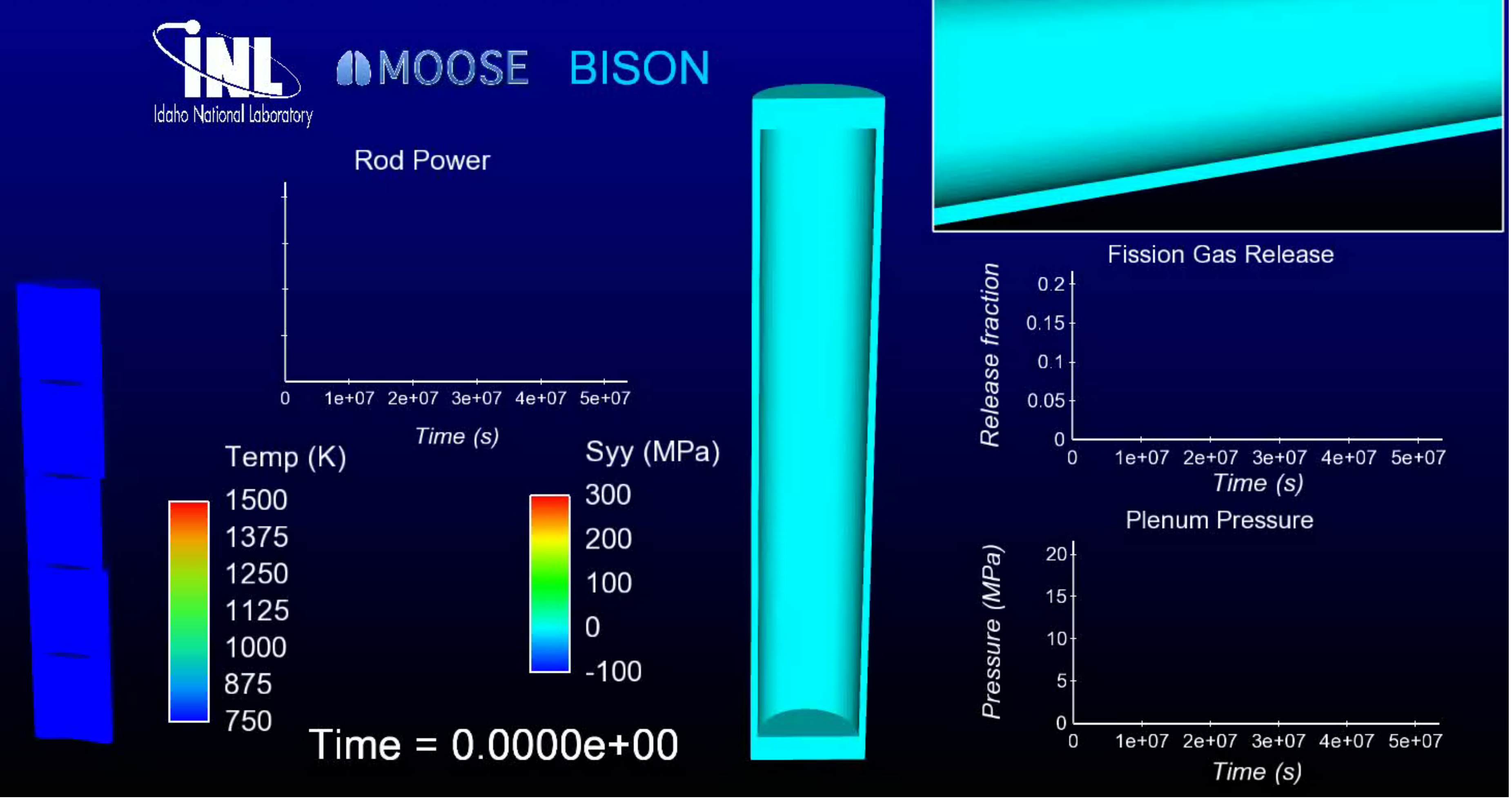
- PCI limits reactor performance associated with power uprates, higher burnup and manufacturing quality assurance around missing pellet surface (MPS) chips and operating flexibility during power changes
- 3-D fuel performance model is critical to assess complex, coupled physics and irregular geometries responsible for PCI fuel failures and poor reactor performance



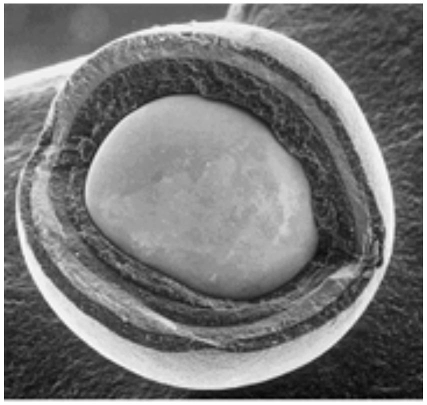


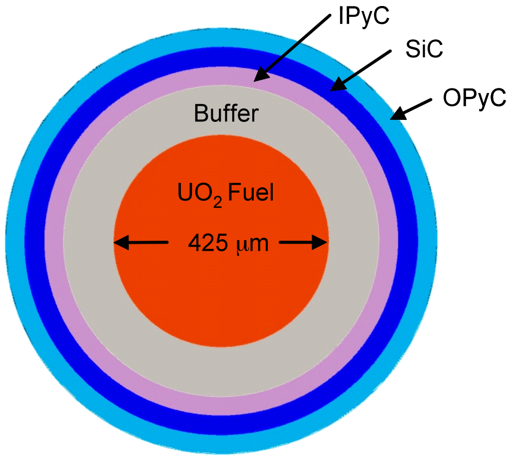
Figures from Robert Montgomery (Anatech)

Missing Pellet Surface

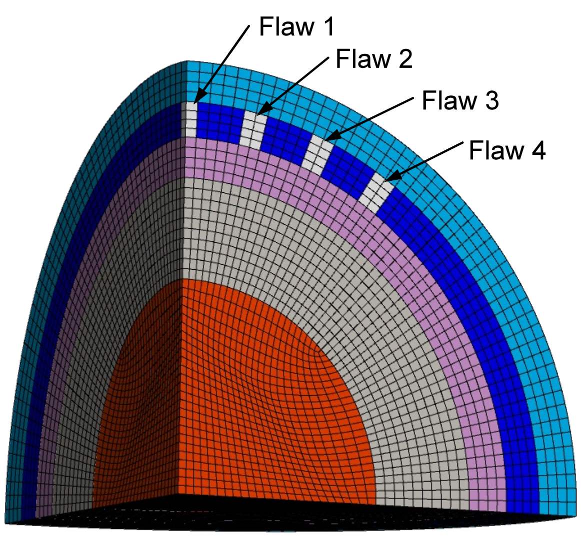


TRISO Fuel Particle Model

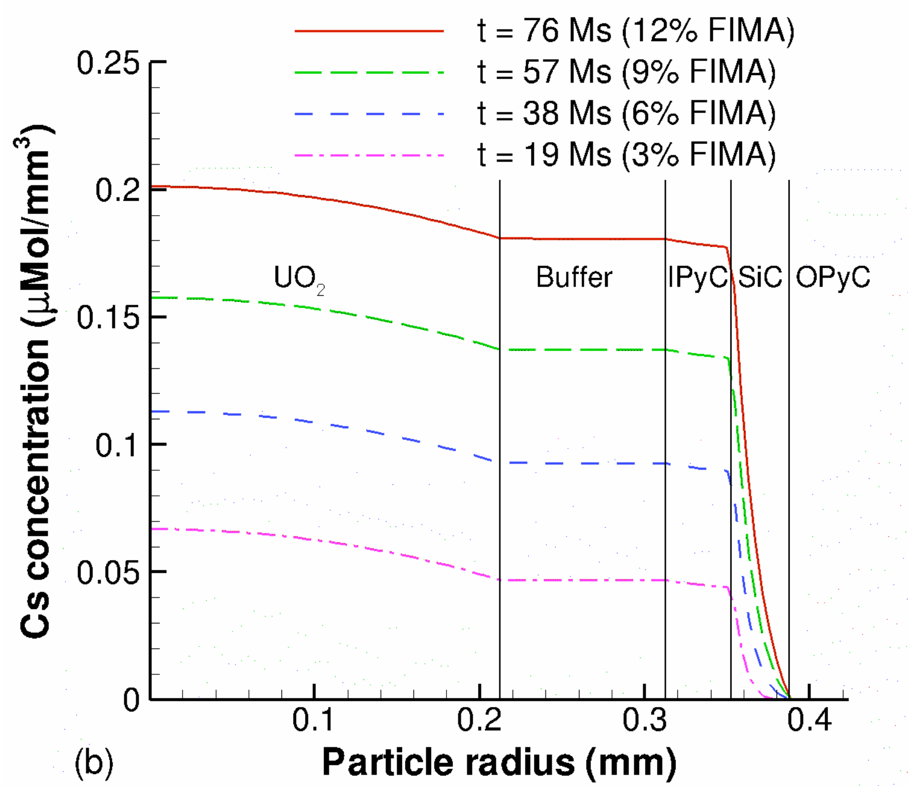


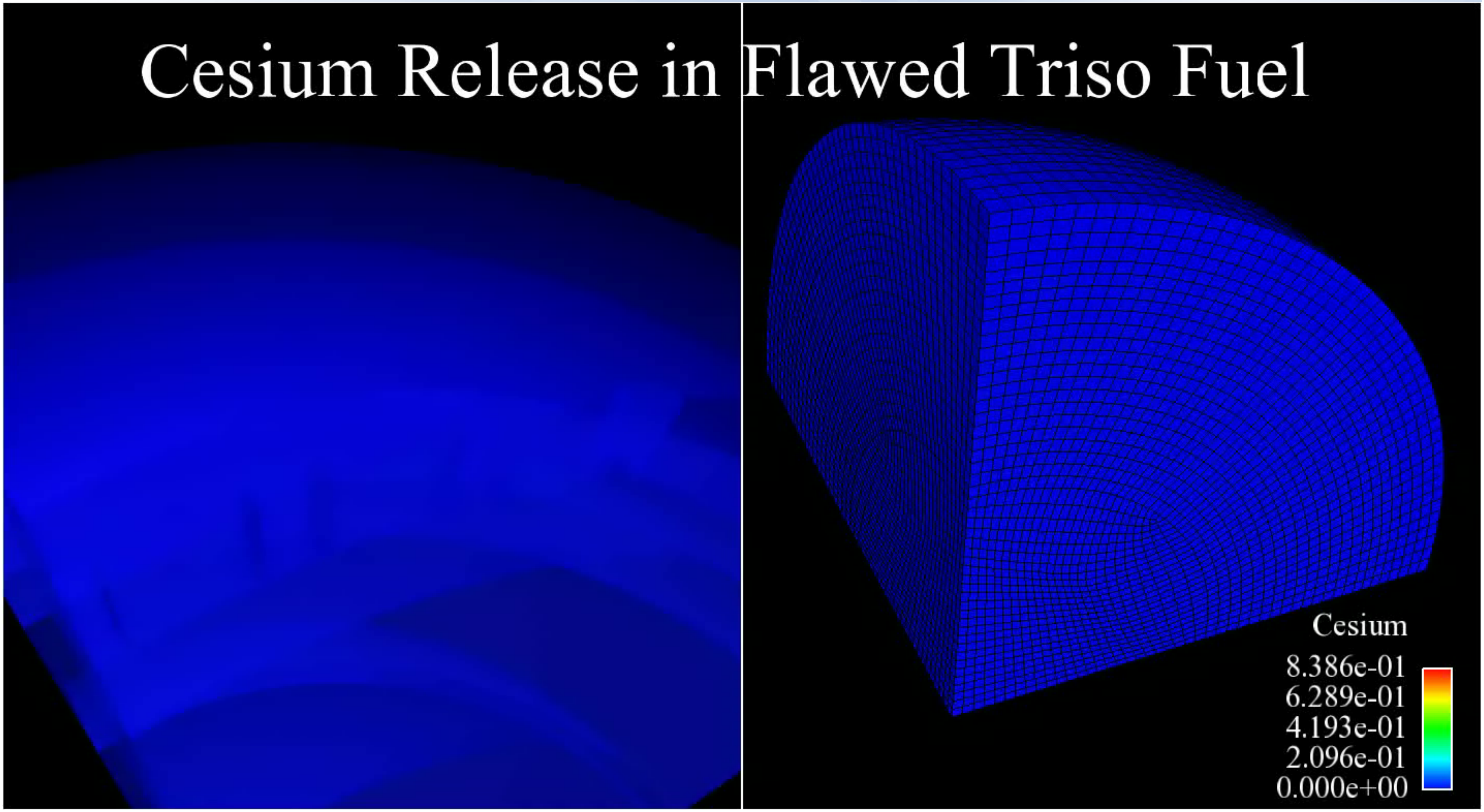


- Gen IV helium-cooled thermal reactor
- Fission product release is a concern



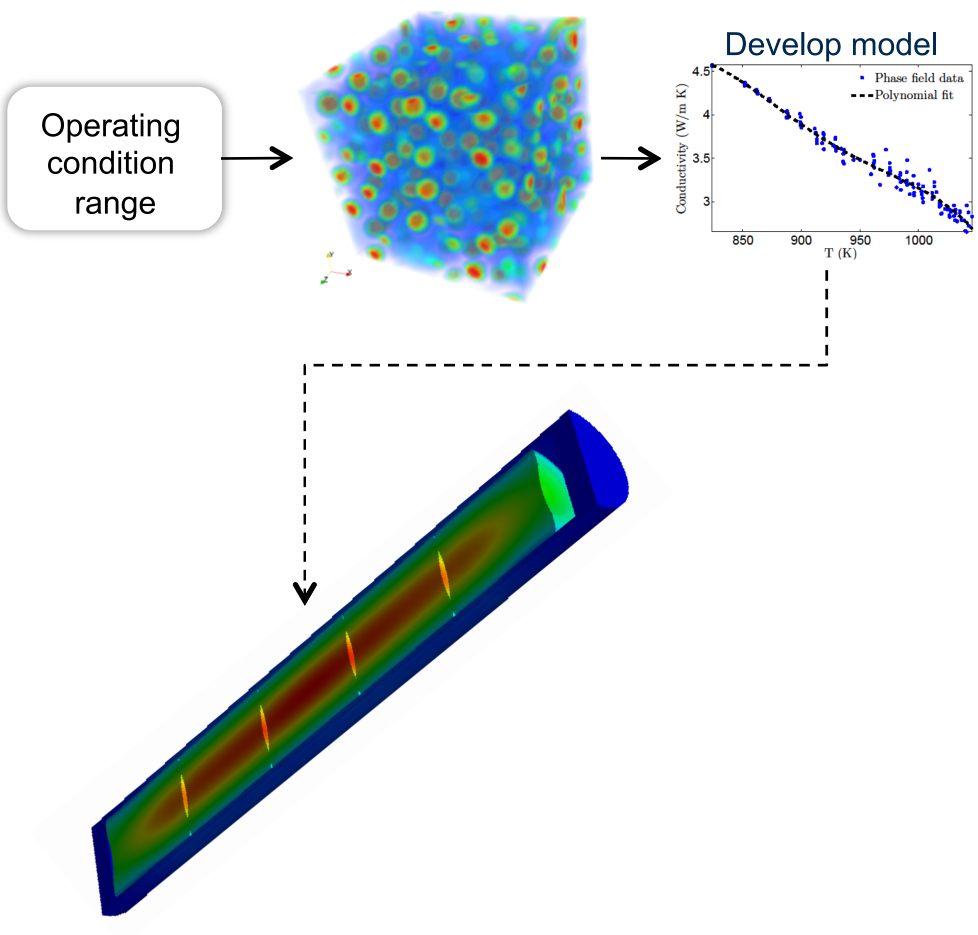
Flaws in the SiC layer have a large effect on fission gas release



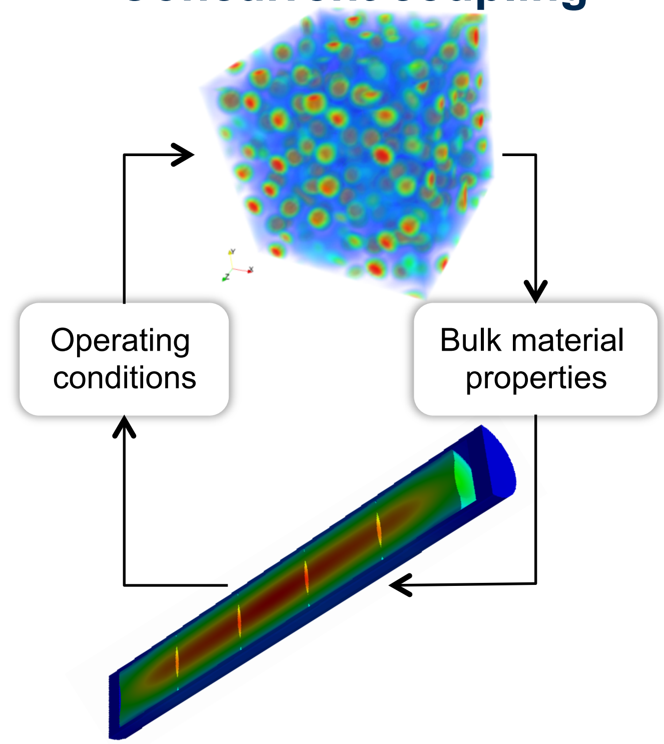

Cesium Release in Flawed Triso Fuel
Cesium
8.386e-01
6.289e-01
4.193e-01
2.096e-01
0.000e+00

Multiscale Coupling Methods

- Physics-based materials model are developed from the mesoscale simulation results



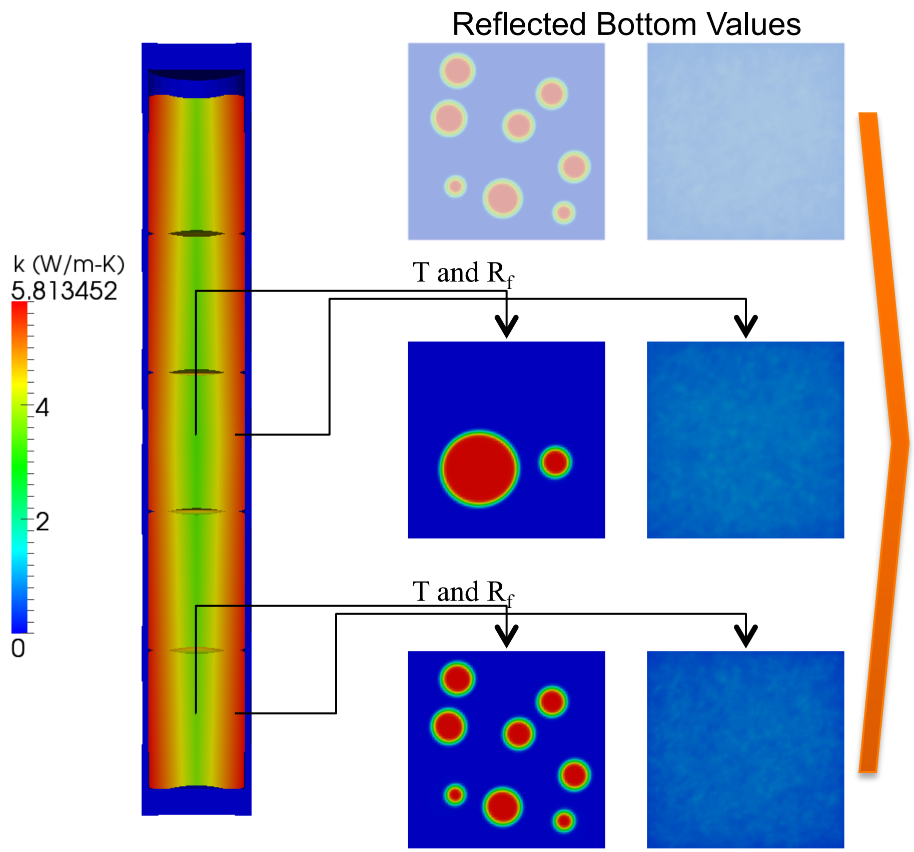
Concurrent coupling



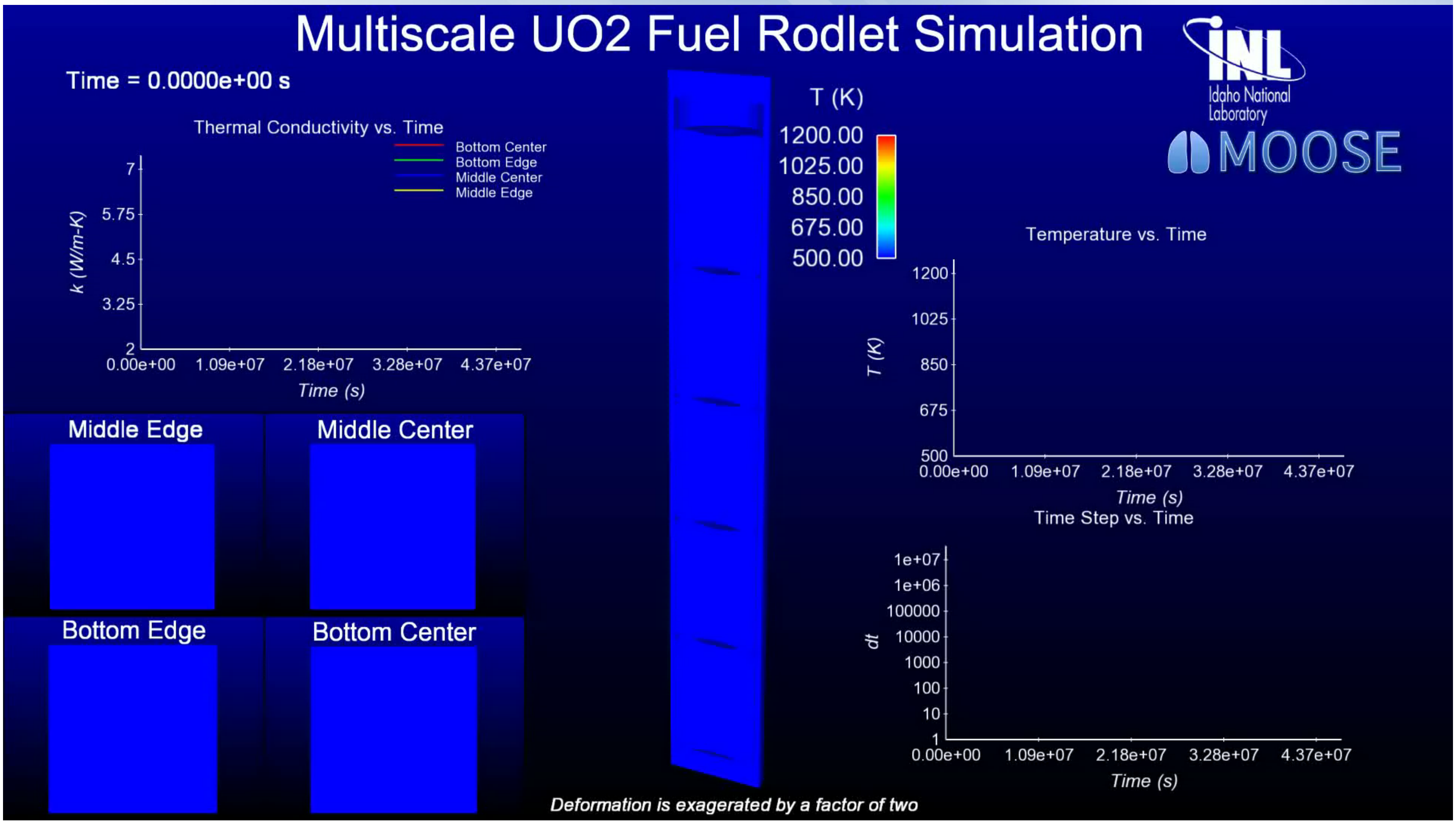
- Another tool for developing materials models
- Captures interaction between the scales
- Can locate important coupled behaviors
- More computationally expensive

Concurrent Coupling Demonstration

- BISON fuel rodlet simulation is coupled to four mesoscale simulations
  - Mesoscale simulation models the effect of voids on thermal conductivity
- Both length scales operate at the same times throughout the simulation



- Temperature and fission rate are passed to mesoscale at four locations.
- Mesoscale thermal conductivity is interpolated throughout the stack
- Bottom values are reflected to the top of the stack for the interpolation

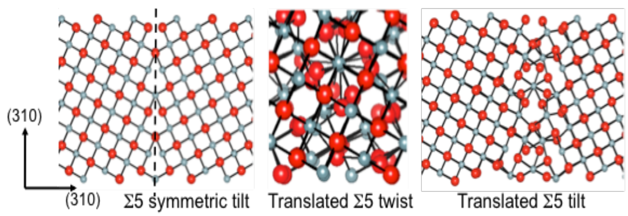

Multiscale UO2 Fuel Rodlet Simulation
Time = 0.0000e+00 s
Thermal Conductivity vs. Time
Bottom Center
Bottom Edge
Middle Center
Middle Edge
k (W/m-K)
7
5.75
4.5
3.25
2
0.00e+00
1.09e+07
2.18e+07
3.28e+07
4.37e+07
Time (s)
Middle Edge
Middle Center
Bottom Edge
Bottom Center
T (K)
1200.00
1025.00
850.00
675.00
500.00
Idaho National Laboratory
MOOSE
Temperature vs. Time
T (K)
1200
1025
850
675
500
0.00e+00
1.09e+07
2.18e+07
3.28e+07
4.37e+07
Time (s)
Time Step vs. Time
dt
1e+07
1e+06
100000
10000
1000
100
10
1
0.00e+00
1.09e+07
2.18e+07
3.28e+07
4.37e+07
Time (s)
Deformation is exagerated by a factor of two

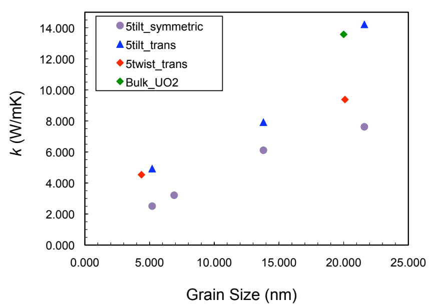
Material Model Example

- Typical models of the effect of porosity on thermal conductivity assume a random bubble distribution, however, bubbles often form on grain boundaries

Atomistic

- The UO_2 grain boundary thermal resistance is calculated using MD simulation for three GB types





Boundary Type	Grain size (nm)	k (W/mK)	R_k (m^2K/W)
Symmetry Σ5 tilt	21.6	7.62	56
Translated Σ5 twist	21.6	14.22	20.13
Translated Σ5 tilt	20.24	9.38	39

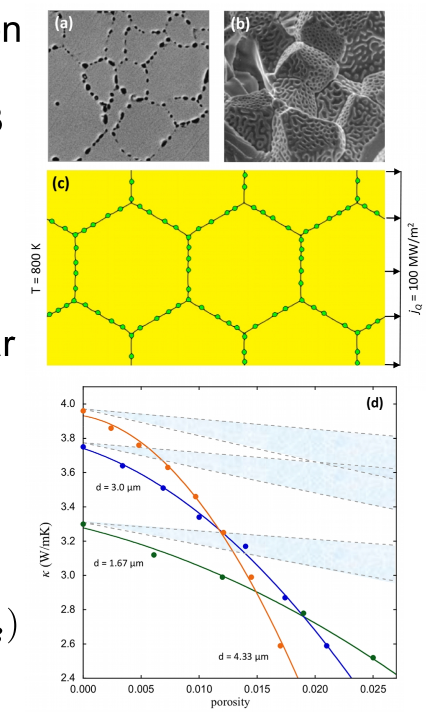
Mesoscale

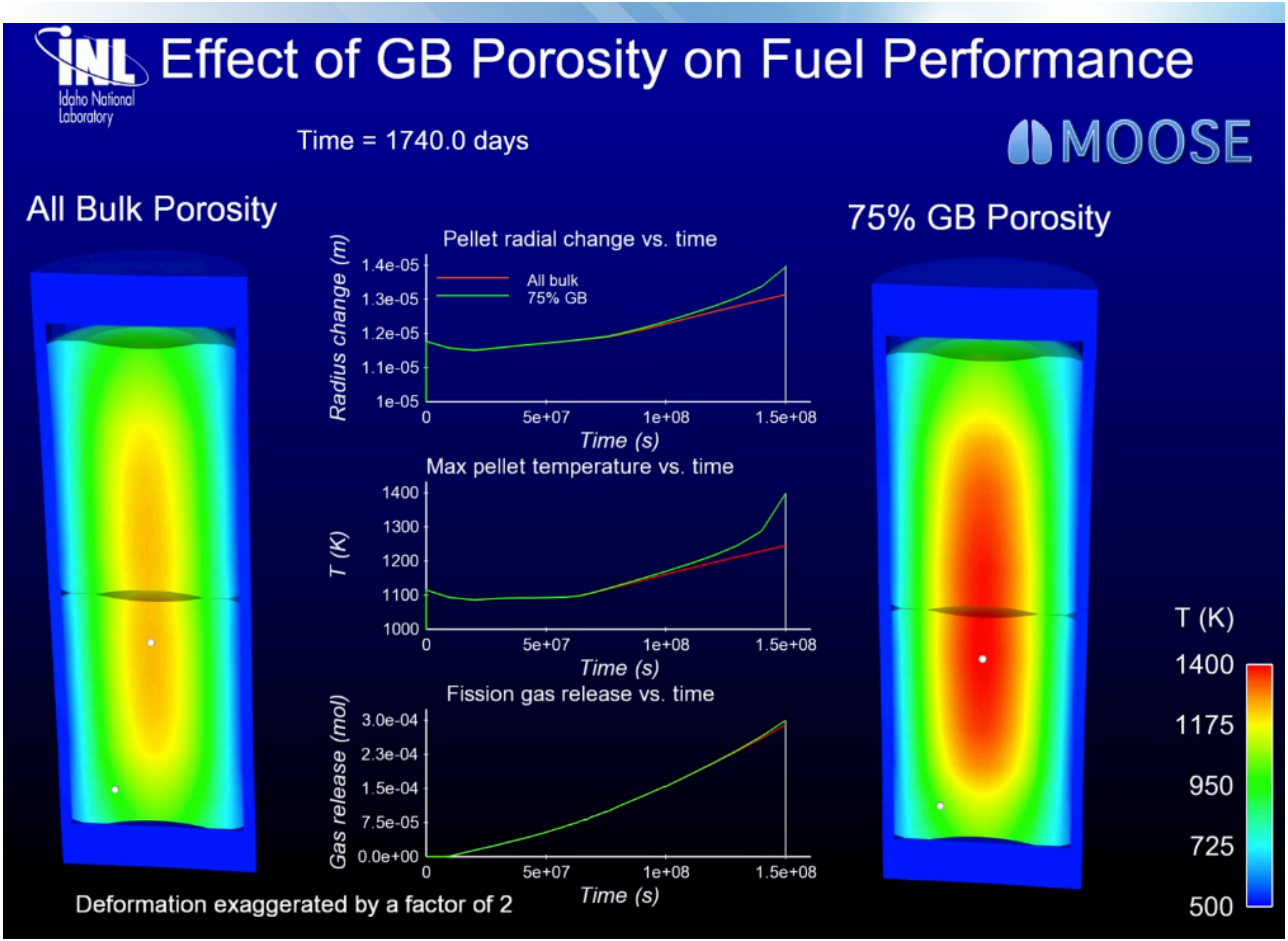
- Mesoscale heat conduction simulations are used to determine the effect of GB porosity on thermal conductivity

- An expression of the k multiplier with intergranular porosity as a function of grain size d and grain boundary coverage using the GB thermal resistance from atomistic

$$R'_k = A + (R^0_k - A)(1 - X^C_{GB})$$

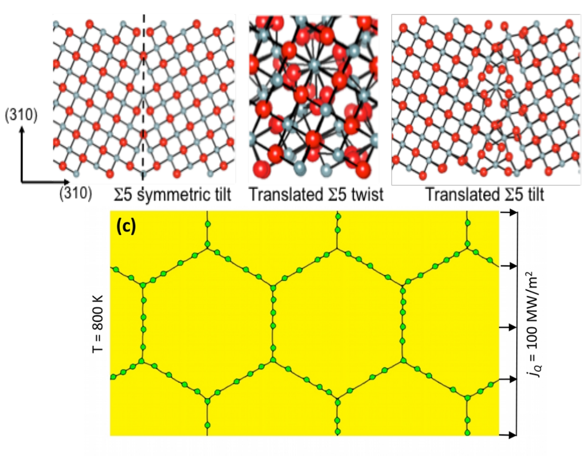
$$f_{GB} = \frac{\kappa_0}{1+\kappa_0 R'_k/d}$$

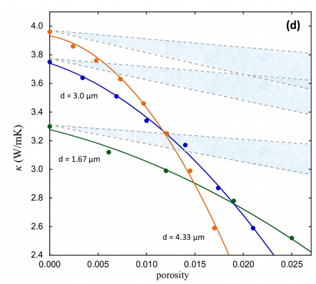



Idaho National Laboratory
Effect of GB Porosity on Fuel Performance
Time = 1740.0 days
MOOSE
All Bulk Porosity
75% GB Porosity
Pellet radial change vs. time
Radius change (m)
1.4e-05
1.3e-05
1.2e-05
1.1e-05
1e-05
All bulk
75% GB
0
5e+07
1e+08
1.5e+08
Time (s)
Max pellet temperature vs. time
T (K)
1400
1300
1200
1100
1000
0
5e+07
1e+08
1.5e+08
Time (s)
Fission gas release vs. time
Gas release (mol)
3.0e-04
2.3e-04
1.5e-04
7.5e-05
0.0e+00
0
5e+07
1e+08
1.5e+08
Time (s)
T (K)
1400
1175
950
725
500
Deformation exaggerated by a factor of 2

Conclusions

- Radiation-induced microstructure evolution has a large effect on fuel performance
- Multiscale modeling in conjunction with separate effects and integrated testing provide a means of developing more predictive fuel performance models





$$R'_k = A + (R^0_k - A)(1 - X^C_{GB})$$